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PASADENA, CALIFORNIA 91109

ENVIRONMENTAL QUALITY LABORATORY

Department of Energy
Institutional Grant to the
California Institute of Technology
Environmental Quality Laboratory Block

Progress Report on Project Element No. 6

December 1, 1977 - November 30, 1978

RELATION OF EMISSIONS TO AIR QUALITY
FOR PHOTOCHEMICAL SMOG

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EQL Open File Report No. 79-7

February 1979



Relation of Emissions to Air Quality for Photochemical Smog

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Effective evaluation of air pollution control strategies requires the use of validated and reliable mathematical models that can relate pollutant emissions to atmospheric air quality. The primary objective of this research program has been to develop a fundamental modeling capability to assess the effectiveness of air pollution control measures in reducing smog. An important aspect of the development has been to simplify the preparation of input data and operational use of the resulting model. The system has been designed to be used by air pollution agencies with relatively little experience in atmospheric physics and chemistry. The assumptions commonly employed in model formulations have been evaluated to ensure a valid representation of the physical and chemical processes in the atmosphere.

As part of this project a new set of objective analysis procedures has been developed to generate meteorological fields from sparse and discrete surface level observations (Publications 6a and 6b). New parameterizations of turbulent diffusivity and surface interactions have led to a better understanding of the mixing and removal of chemically reacting pollutants. Numerical techniques have been developed to solve the large system of coupled nonlinear partial differential equations which describe the pollutant transport and chemical reactions.

*Former investigator who has left Caltech.

A new chemical mechanism, incorporating the latest information on reaction paths and rate data, has been developed. The mechanism has been extensively and successfully tested against smog chamber experiments. Additional studies have been completed to assess the sensitivity of the mechanism's predictions to uncertainties in such parameters as rate constants and initial conditions.

A summary of the results of the work completed to date was presented at the recent Conference on Atmospheric Turbulence, Diffusion and Air Quality sponsored by the American Meteorological Society (Publication 6c). The results will be presented in detail in a forthcoming Environmental Quality Laboratory Report (Publication 6d).

This research on relating emissions of air pollutants to atmospheric concentrations will be continued by Professor John H. Seinfeld and Mr. Gregory J. McRae by undertaking the following tasks:

1. Continue validation of the airshed model, developed under the initial phase, against data available in the South Coast Air Basin of Southern California. This task will be undertaken in collaboration with the California Air Resources Board, Air Quality Modeling Section.
2. Examine the sensitivity of the model predictions to uncertainties in meteorological parameters, emissions rates and initial pollutant distributions. This work will involve application of a new technique, the Fourier Amplitude Sensitivity Test, for sensitivity analysis (Publications 6e and 6f).
3. Employ the validation results and the new lumped chemical mechanism in an assessment of the ozone isopleth modeling technique.

Although the model application is site specific, there will be important research results applicable for other air pollution problems, especially those involving reacting species. In fact, it is impossible to make practical progress in air pollution modeling without being site specific to learn how to cope with all the real world problems (Such as inadequate or inconsistent input data). Partial sponsorship by DOE and interactions with DOE researchers will assist in the dissemination and exchange of necessary skills. An adequate ability to predict regional air quality consequences is, of course, an important part of assessing the environmental impact of various energy supply strategies.

PUBLICATIONS FROM PROJECT ELEMENT NO. 6

- 6a. Goodin, W.R., G.J. McRae and J.H. Seinfeld, "A Comparison of Interpolation Methods for Sparse Data: Application to Wind and Concentration Fields," Journal of Applied Meteorology (accepted for publication), 1979.
6. Goodin, W.R., G.J. McRae and J.H. Seinfeld, "An Objective Analysis Technique for Constructing Three-dimensional Urban-Scale Wind Fields," Journal of Applied Meteorology (to be submitted for publication), 1979.
- * 6c. McRae, G.J., W.R. Goodin and J.H. Seinfeld, "Development of a Second-Generation Airshed Model for Photochemical Air Pollution," Proceedings, Fourth Conference on Atmospheric Turbulence, Diffusion and Air Quality, Reno, Nevada, January 15-18, 1979. American Meteorological Society.
- 6d. McRae, G.J., W.R. Goodin and J.H. Seinfeld, "Mathematical Modeling of Photochemical Air Pollution," Environmental Quality Laboratory Report, California Institute of Technology, Pasadena, California (to be published), 1979 (approximately 800 pages).
- * 6e. Fall, A.H., G.J. McRae and J.H. Seinfeld, "Sensitivity and Uncertainty of Reaction Mechanisms for Photochemical Air Pollution," International Journal of Chemical Kinetics (accepted for publication), 1978.
- * 6f. Koda, M., G.J. McRae and J.H. Seinfeld, "Automatic Sensitivity Analysis of Kinetic Mechanisms," International Journal of Chemical Kinetics (in press), 1978.

* Asterisks denote publications containing work not sponsored directly by DOE.